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Percolation processes in three dimensions

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Abstract. The derivation of low-density series expansions for the mean cluster size in random site and bond mixtures on a three-dimensional lattice is described briefly. New data are given for the face-centred cubic, body-centred cubic, simple cubic and diamond lattices. The critical concentration for the site problem is estimated as $p_c = 0{\cdot}198 \pm 0{\cdot}003$ (FCC), $p_c = 0{\cdot}245 \pm 0{\cdot}004$ (BCC), $p_c = 0{\cdot}310 \pm 0{\cdot}004$ (SC), $p_c = 0{\cdot}428 \pm 0{\cdot}004$ (D); for the bond problem as $p_c = 0{\cdot}119 \pm 0{\cdot}001$ (FCC), $p_c = 0{\cdot}1785 \pm 0{\cdot}002$ (BCC), $p_c = 0{\cdot}247 \pm 0{\cdot}003$ (SC), $p_c = 0{\cdot}388 \pm 0{\cdot}005$ (D). It is concluded that the data are reasonably consistent with the hypothesis that the mean cluster size $S(p) \simeq C(p_c - p)^{-\gamma}$ as $p \to p_c-$ with γ a dimensional invariant, $\gamma = 1{\cdot}66 \pm 0{\cdot}07$ in three dimensions. Estimates of the critical amplitude C are also given.

1. Introduction

In this paper we describe briefly the derivation and analysis of series expansions required for a study of random mixtures of sites (or bonds) on a three-dimensional lattice. We have described the theoretical background and introduced the series method in earlier papers (Sykes and Glen 1976, Sykes *et al* 1976a,b,c to be referred to as I–IV). Our objectives are to estimate the critical concentration for the more usual three-dimensional lattices and to investigate the hypothesis (Sykes and Essam 1964) that the critical index for the mean cluster size is a dimensional invariant. Explicitly we investigate the hypothesis that

$$S(p) \simeq C(p_c - p)^{-\gamma}, \qquad p \to p_c-. \tag{1.1}$$

In II we concluded that for *two*-dimensional lattices

$$\gamma = 2{\cdot}43 \pm 0{\cdot}03. \tag{1.2}$$

We shall not examine the high density region since a pilot investigation (Sykes *et al* 1976d) has led us to conclude that except for the face-centred cubic lattice it is very difficult to draw firm conclusions with the data currently available.

2. Series expansions for the mean cluster size at low densities

2.1. Site problem

The method described in I § 2 (based on the techniques proposed by Domb (1959) and Martin (1974)) is immediately applicable without modification to a three-dimensional lattice. We have derived *perimeter polynomials*, $D_s(q)$ as defined in I, through D_9 for the face-centred cubic lattice, through D_{10} for the body-centred cubic lattice, through D_{11} for the simple cubic lattice and through D_{14} for the diamond lattice. The rapid growth of the total number of clusters with increasing number of sites restricts the number of perimeter polynomials that can be obtained from a reasonable expenditure of computer time. The asymptotic behaviour of the total number of connected clusters appears to be approximately represented by

$$D_s(1) \simeq As^{-\theta}\lambda^s. \tag{2.1}$$

(For a theoretical justification of the presence of a factor λ^s in (2.1) see Klarner (1967).) From a Padé approximant and ratio analysis (Gaunt and Guttmann 1974) we estimate that θ is about 3/2 and the corresponding indicated values of the cluster growth parameter (λ) are:

$$\begin{aligned} &\text{FCC} && \lambda = 13{\cdot}95 \pm 0{\cdot}08 \\ &\text{BCC} && \lambda = 11{\cdot}19 \pm 0{\cdot}06 \\ &\text{SC} && \lambda = 8{\cdot}35 \pm 0{\cdot}04 \\ &\text{D} && \lambda = 5{\cdot}54 \pm 0{\cdot}03. \end{aligned} \tag{2.2}$$

In two dimensions $\theta \simeq 1$ (I § 2) and estimates of two-dimensional growth parameters are given in equation (2.4) of I.

We give the values of the perimeter polynomials in the appendix. From them the mean size of clusters at low densities

$$S(p) = \sum_r b_r p^r \tag{2.3}$$

follows by the method of I. An extra coefficient would be obtained if the corresponding expansion for the mean number of clusters were available to the appropriate order but in practice this is quite difficult to derive. We give the values of the b_r in table 1(a).

2.2. *Bond problem*

By direct machine enumeration we have derived perimeter polynomials for the bond problem through D_7 for the face-centred cubic lattice, through D_8 for the body-centred cubic lattice, through D_9 for the simple cubic lattice and through D_{12} for the diamond lattice. As in two dimensions the cluster growth parameters in (2.1) are larger than those for the corresponding site mixtures:

$$\begin{aligned} &\text{FCC} && \lambda = 23{\cdot}80 \pm 0{\cdot}20 \\ &\text{BCC} && \lambda = 15{\cdot}25 \pm 0{\cdot}10 \\ &\text{SC} && \lambda = 10{\cdot}62 \pm 0{\cdot}06 \\ &\text{D} && \lambda = 6{\cdot}13 \pm 0{\cdot}03. \end{aligned} \tag{2.4}$$

For bond mixtures the series expansion for the mean number of clusters is readily obtained from the number of weak embeddings of linear (star) graphs in the lattice. The technique is described in detail by Essam and Sykes (1966) and we have added an extra term to the expansion of $S(p)$ in every case. The additional weak k weights required are given by Heap (1966). We give the coefficients b_r corresponding to the bond problem in table 1(b).

Table 1. Coefficients for expansion of $S(p)=\Sigma_r b_r p^r$.

r	Face-centred	Body-centred	Simple cubic	Diamond
(*a*) Site problem				
1	12	8	6	4
2	84	56	30	12
3	504	248	114	36
4	3012	1232	438	108
5	17142	5690	1542	264
6	96 228†	26 636	5754	708
7	532 028†	113 552	19 574	1668
8	2 918 388†	532 736†	71 958	4536
9	15 763 866†	2 207 108†	233 574†	10 926
10		10 385 062†	870 666†	28 416
11			2 696 274†	67 824†
12				172 464†
13				408 484†
14				1 035 932†
(*b*) Bond problem				
1	22	14	10	6
2	234	98	50	18
3	2348	650	238	54
4	22 726	4202	1114	162
5	214 642	26 162	4998	456
6	1 993 002	163 154	22 562	1302
7	18 266 276†	984 104	98 174	3630
8	165 688 208†	6 015 512	434 894	10 158
9		35 540 288†	1 855 346	27 648
10			8 125 390†	77 022
11				206 508
12				570 072†
13				1 521 822†

† New coefficient.

3. Analysis of series

To study the expansions for $S(p)$ given in table 1(*a*) and (*b*) we have followed procedures similar to those described in II § 2 for the two-dimensional lattices. In general the series are not sufficiently well behaved with the number of coefficients at present available, to provide anything more than rather rough estimates of the critical parameters. For this reason we omit the details of the standard ratio and Padé approximant analyses and simply present the results.

Convergence appears to be best for the bond problem on the face-centred cubic lattice and we estimate by Dlog Padé and ratio techniques that

$$p_c = 0{\cdot}119 \pm 0{\cdot}001 \qquad \text{FCC(B)}. \tag{3.1}$$

This estimate is in good agreement with recent evidence from other sources. For example, Essam *et al* (1976) obtained exactly the same result from an analysis of the moments of the cluster size distribution. Dunn *et al* (1975) found that a more precise estimate may be obtained from the second moment of the pair connectedness and concluded that

$$p_c = 0{\cdot}1190 \pm 0{\cdot}0005 \qquad \text{FCC(B)}. \tag{3.2}$$

The poles of the Padé approximants to $(\mathrm{d}/\mathrm{d}p) \ln S(p)$ plotted against the corresponding residues define quite accurately a single smooth curve (or pole–residue plot) from which we obtain the estimate

$$\gamma = 1{\cdot}66 \pm 0{\cdot}02 + 90\Delta p_c. \tag{3.3}$$

Assuming $|\Delta p_c| \leqslant 0{\cdot}001$, corresponding to (3.1), then (3.3) gives

$$\gamma = 1{\cdot}66 \pm 0{\cdot}11. \tag{3.4}$$

Assuming instead $|\Delta p_c| \leqslant 0{\cdot}0005$ corresponding to (3.2) we obtain

$$\gamma = 1{\cdot}66 \pm 0{\cdot}07. \tag{3.5}$$

The series for the other three-dimensional mixtures are not inconsistent with $\gamma = 1{\cdot}66$ but we have found it difficult to draw any more precise conclusions. The same estimate as (3.5) was obtained recently by Essam *et al* (1976) while Dunn *et al* (1975) (using the mean size defined by site content) obtained $\gamma = 1{\cdot}70 \pm 0{\cdot}11$. Monte Carlo estimates include $\gamma = 1{\cdot}8 \pm 0{\cdot}05$ (Kirkpatrick 1976) and $\gamma = 1{\cdot}6 \pm 0{\cdot}1$ (Sur *et al* 1976, private communication). Our estimate (3.5) lies well within the uncertainty limits of all other estimates except that due to Kirkpatrick.

Making the not unreasonable assumption that γ is a dimensional invariant, as it seems to be in two dimensions (see II), we have used the estimate (3.4) to obtain more precise (although 'biased') estimates of p_c, namely

$$\begin{aligned} p_c &= 0{\cdot}1785 \pm 0{\cdot}002 && \text{BCC(B)} \\ p_c &= 0{\cdot}247 \pm 0{\cdot}003 && \text{SC(B)} \\ p_c &= 0{\cdot}388 \pm 0{\cdot}005 && \text{D(B)} \end{aligned} \tag{3.6}$$

and

$$\begin{aligned} p_c &= 0{\cdot}198 \pm 0{\cdot}003 && \text{FCC(S)} \\ p_c &= 0{\cdot}245 \pm 0{\cdot}004 && \text{BCC(S)} \\ p_c &= 0{\cdot}310 \pm 0{\cdot}004 && \text{SC(S)} \\ p_c &= 0{\cdot}428 \pm 0{\cdot}004 && \text{D(S)}. \end{aligned} \tag{3.7}$$

The central estimates in (3.6) are identical (to the first three decimal places) with those given by Sykes and Essam (1964); our uncertainties are rather smaller in general. For the site problems we have three or four more coefficients than were available to Sykes and Essam and our central estimates in (3.7) are some 0·002 or 0·003 higher than theirs and have smaller uncertainties. For the simple cubic site problem recent Monte Carlo work has given $p_c = 0{\cdot}312 \pm 0{\cdot}001$ (Kirkpatrick 1976) and $p_c = 0{\cdot}3115 \pm 0{\cdot}0005$ (Sur *et al*, private communication) in good agreement with (3.7).

We have used the central estimates of p_c together with $\gamma = 1{\cdot}66$ to estimate, by the usual Padé methods, the critical amplitude C defined by (1.1). Our results are

$$\begin{array}{ll} 0{\cdot}041 \pm 0{\cdot}001 & \textsc{fcc(b)} \\ 0{\cdot}074 \pm 0{\cdot}001 & \textsc{bcc(b)} \\ 0{\cdot}122 \pm 0{\cdot}001 & \textsc{sc(b)} \\ 0{\cdot}222 \pm 0{\cdot}002 & \textsc{d(b)} \end{array} \tag{3.8}$$

and

$$\begin{array}{ll} 0{\cdot}101 \pm 0{\cdot}001 & \textsc{fcc(s)} \\ 0{\cdot}142 \pm 0{\cdot}001 & \textsc{bcc(s)} \\ 0{\cdot}185 \pm 0{\cdot}002 & \textsc{sc(s)} \\ 0{\cdot}261 \pm 0{\cdot}005 & \textsc{d(s)}. \end{array} \tag{3.9}$$

The uncertainties in p_c and in γ each introduce additional uncertainties in C of about

$$+4{\cdot}9\Delta p_c - 2{\cdot}1 p_c \Delta\gamma. \tag{3.10}$$

For both site and bond mixtures the amplitudes are seen to decrease monotonically with increasing lattice coordination number, in agreement with the Bethe approximation (Fisher and Essam 1961). It seems that on a given lattice the amplitude for the bond problem is always less than for the corresponding site problem. The opposite is true in the Bethe approximation.

4. Conclusions

Although we have found it very difficult to draw precise conclusions, all the available series appear to be reasonably consistent with the hypothesis that γ is a dimensional invariant for both bond and site mixtures in three dimensions. Our best estimate of $\gamma = 1{\cdot}66 \pm 0{\cdot}07$ is close to $1\frac{2}{3}$ and we adopt this simple fraction as a convenient mnemonic to replace the earlier tentative value of $1\frac{11}{16} (= 1{\cdot}6875)$ of Sykes and Essam (1964).

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Appendix. Perimeter polynomials for the site problem

Face-centred cubic lattice

$D_1 = q^{12} \qquad D_2 = 6q^{18} \qquad D_3 = 8q^{22} + 12q^{23} + 30q^{24}$

$D_4 = 2q^{24} + 27q^{26} + 48q^{27} + 96q^{28} + 144q^{29} + 158q^{30}$

$D_5 = 24q^{28} + 6q^{29} + 132q^{30} + 264q^{31} + 423q^{32} + 780q^{33} + 1194q^{34} + 1212q^{35} + 846q^{36}$

$$D_6=6q^{30}+24q^{31}+145q^{32}+168q^{33}+914q^{34}+1308q^{35}+2688q^{36}+5000q^{37}$$
$$+7140q^{38}+10\,272q^{39}+11\,340q^{40}+9168q^{41}+4662q^{42}$$
$$D_7=36q^{33}+80q^{34}+288q^{35}+1220q^{36}+1968q^{37}+5382q^{38}+10\,308q^{39}+18\,918q^{40}$$
$$+31\,128q^{41}+53\,616q^{42}+75\,528q^{43}+93\,852q^{44}+110\,680q^{45}$$
$$+98\,496q^{46}+65\,700q^{47}+26\,182q^{48}$$
$$D_8=24q^{35}+58q^{36}+576q^{37}+1098q^{38}+3336q^{39}+10\,176q^{40}+17\,712q^{41}$$
$$+42\,672q^{42}+77\,862q^{43}+140\,142q^{44}+244\,659q^{45}+389\,142q^{46}$$
$$+575\,652q^{47}+802\,362q^{48}+980\,484q^{49}+1\,085\,502q^{50}+1\,066\,224q^{51}$$
$$+804\,912q^{52}+456\,888q^{53}+149\,934q^{54}$$
$$D_9=6q^{37}+152q^{38}+504q^{39}+1616q^{40}+6558q^{41}+14\,109q^{42}+36\,068q^{43}$$
$$+85\,875q^{44}+168\,600q^{45}+351\,436q^{46}+635\,168q^{47}+1\,147\,140q^{48}$$
$$+1\,938\,126q^{49}+3\,097\,776q^{50}+4\,684\,860q^{51}+6\,594\,194q^{52}$$
$$+8\,692\,066q^{53}+10\,577\,942q^{54}+11\,507\,324q^{55}+11\,296\,227q^{56}$$
$$+9\,590\,904q^{57}+6\,335\,391q^{58}+3\,124\,172q^{59}+871\,605q^{60}.$$

Body-centred cubic lattice

$D_1=q^8$ $\qquad D_2=4q^{14}$ $\qquad D_3=12q^{17}+12q^{19}+4q^{20}$

$$D_4=42q^{20}+78q^{22}+32q^{23}+36q^{24}+24q^{25}+4q^{26}$$
$$D_5=6q^{21}+152q^{23}+30q^{24}+408q^{25}+182q^{26}+384q^{27}+336q^{28}+144q^{29}$$
$$+108q^{30}+36q^{31}+4q^{32}$$
$$D_6=51q^{24}+24q^{25}+632q^{26}+204q^{27}+2088q^{28}+1352q^{29}+2748q^{30}+2568q^{31}$$
$$+2112q^{32}+2016q^{33}+1044q^{34}+480q^{35}+216q^{36}+48q^{37}+4q^{38}$$
$$D_7=12q^{25}+16q^{26}+324q^{27}+144q^{28}+3096q^{29}+2058q^{30}+10\,416q^{31}+8774q^{32}$$
$$+18\,408q^{33}+18\,438q^{34}+20\,884q^{35}+20\,820q^{36}+15\,024q^{37}$$
$$+11\,184q^{38}+6756q^{39}+2820q^{40}+1148q^{41}+360q^{42}+60q^{43}+4q^{44}$$
$$D_8=8q^{26}+102q^{28}+96q^{29}+2316q^{30}+1956q^{31}+16\,002q^{32}+15\,192q^{33}+56\,142q^{34}$$
$$+57\,196q^{35}+119\,664q^{36}+132\,588q^{37}+169\,858q^{38}+179\,238q^{39}$$
$$+164\,856q^{40}+147\,638q^{41}+107\,388q^{42}+67\,320q^{43}+40\,276q^{44}$$
$$+18\,432q^{45}+6780q^{46}+2256q^{47}+540q^{48}+72q^{49}+4q^{50}$$
$$D_9=q^{26}+48q^{29}+1320q^{31}+1448q^{32}+15\,186q^{33}+18\,228q^{34}+90\,048q^{35}$$
$$+106\,470q^{36}+325\,710q^{37}+390\,862q^{38}+773\,976q^{39}+929\,610q^{40}$$
$$+1\,288\,146q^{41}+1\,460\,972q^{42}+1\,536\,180q^{43}+1\,518\,148q^{44}$$
$$+1\,295\,178q^{45}+1\,027\,578q^{46}+734\,684q^{47}+440\,454q^{48}+240\,324q^{49}$$
$$+116\,266q^{50}+44\,280q^{51}+14\,196q^{52}+3912q^{53}+756q^{54}+84q^{55}+4q^{56}$$

$$D_{10}=6q^{29}+12q^{31}+770q^{32}+480q^{33}+12\,072q^{34}+16\,552q^{35}+101\,292q^{36}+149\,064q^{37}+552\,824q^{38}+763\,944q^{39}+2\,000\,136q^{40}+2\,685\,656q^{41}+5\,107\,226q^{42}+6\,584\,694q^{43}+9\,491\,284q^{44}+11\,426\,458q^{45}+13\,115\,682q^{46}+14\,005\,452q^{47}+13\,476\,452q^{48}+12\,123\,168q^{49}+9\,883\,164q^{50}+7\,239\,324q^{51}+4\,900\,860q^{52}+2\,923\,840q^{53}+1\,521\,540q^{54}+720\,672q^{55}+290\,912q^{56}+95\,808q^{57}+26\,880q^{58}+6224q^{59}+1008q^{60}+96q^{61}+4q^{62}.$$

Simple cubic lattice

$D_1=q^6 \qquad D_2=3q^{10} \qquad D_3=12q^{13}+3q^{14}$

$$D_4=8q^{15}+51q^{16}+24q^{17}+3q^{18}$$

$$D_5=12q^{17}+99q^{18}+228q^{19}+156q^{20}+36q^{21}+3q^{22}$$

$$D_6=6q^{18}+280q^{20}+732q^{21}+1128q^{22}+960q^{23}+324q^{24}+48q^{25}+3q^{26}$$

$$D_7=q^{18}+72q^{21}+662q^{22}+2496q^{23}+4990q^{24}+6432q^{25}+5682q^{26}+2564q^{27}+540q^{28}+60q^{29}+3q^{30}$$

$$D_8=12q^{21}+6q^{22}+288q^{23}+2089q^{24}+8340q^{25}+20\,316q^{26}+33\,312q^{27}+39\,312q^{28}+34\,635q^{29}+18\,456q^{30}+5256q^{31}+816q^{32}+72q^{33}+3q^{34}$$

$$D_9=48q^{23}+90q^{24}+1284q^{25}+7415q^{26}+30\,600q^{27}+79\,512q^{28}+154\,936q^{29}+226\,509q^{30}+250\,476q^{31}+217\,704q^{32}+128\,460q^{33}+45\,285q^{34}+9312q^{35}+1152q^{36}+84q^{37}+3q^{38}$$

$$D_{10}=212q^{25}+753q^{26}+5224q^{27}+32\,084q^{28}+115\,836q^{29}+323\,100q^{30}+690\,028q^{31}+1\,163\,910q^{32}+1\,550\,322q^{33}+1\,649\,106q^{34}+1\,405\,920q^{35}+884\,058q^{36}+363\,864q^{37}+93\,546q^{38}+15\,128q^{39}+1548q^{40}+96q^{41}+3q^{42}$$

$$D_{11}=78q^{26}+788q^{27}+4476q^{28}+27\,564q^{29}+134\,622q^{30}+485\,724q^{31}+1\,347\,336q^{32}+3\,077\,772q^{33}+5\,692\,578q^{34}+8\,618\,172q^{35}+10\,775\,094q^{36}+11\,069\,256q^{37}+9\,316\,278q^{38}+6\,083\,556q^{39}+2\,805\,054q^{40}+858\,312q^{41}+172\,794q^{42}+22\,980q^{43}+2004q^{44}+108q^{45}+3q^{46}.$$

Diamond lattice

$D_1=q^4 \qquad D_2=2q^6 \qquad D_3=6q^8 \qquad D_4=22q^{10}$

$D_5=12q^{11}+79q^{12} \qquad D_6=2q^{12}+120q^{13}+276q^{14}$

$$D_7=16q^{13}+66q^{14}+792q^{15}+932q^{16}$$

$$D_8 = 15q^{14} + 184q^{15} + 936q^{16} + 4152q^{17} + 3106q^{18}$$

$$D_9 = 6q^{15} + 292q^{16} + 1872q^{17} + 8152q^{18} + 18\,984q^{19} + 10\,407q^{20}$$

$$D_{10} = 19q^{16} + 336q^{17} + 3876q^{18} + 16\,968q^{19} + 53\,574q^{20} + 80\,400q^{21} + 35\,452q^{22}$$

$$D_{11} = 36q^{17} + 514q^{18} + 6546q^{19} + 39\,114q^{20} + 132\,620q^{21} + 294\,948q^{22} + 329\,652q^{23} + 122\,486q^{24}$$

$$D_{12} = 30q^{18} + 1140q^{19} + 11\,198q^{20} + 82\,362q^{21} + 337\,901q^{22} + 873\,864q^{23} + 1\,476\,224q^{24} + 1\,333\,152q^{25} + 427\,140q^{26}$$

$$D_{13} = 66q^{19} + 1990q^{20} + 22\,884q^{21} + 169\,262q^{22} + 815\,214q^{23} + 2\,502\,843q^{24} + 5\,109\,308q^{25} + 7\,020\,060q^{26} + 5\,345\,004q^{27} + 1\,498\,713q^{28}$$

$$D_{14} = 164q^{20} + 3064q^{21} + 48\,694q^{22} + 365\,082q^{23} + 1\,914\,214q^{24} + 6\,774\,180q^{25} + 16\,403\,034q^{26} + 27\,712\,992q^{27} + 32\,374\,920q^{28} + 21\,256\,836q^{29} + 5\,286\,414q^{30}.$$

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